

A Unified Construction of Variational Methods for the Nonlinear Schrödinger Equation

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Based on an approach introduced by Gerjuoy, Rau, and Spruch, we construct variational principles in a systematic way for the nonlinear Schrödinger equation and obtain new variational principles for the case of Ginzburg-Pitaevskii-Gross equation (GPG) which is believed to describe accurately the Bose-Einstein condensation at zero temperature. As an application of these variational methods, a variational iteration method is proposed for calculating eigenvalue (chemical potential) and wave function for the GPG equation

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1. Introduction

The concept of the Bose-Einstein condensation (BEC) [1] has been known for 73 years, and has been used to describe all physical scales, including liquid ^4He , excitons in semiconductors, pions and kaons in dense nuclear matter (neutron stars, supernovae), and elementary particles [2]. It is only a few years ago that the BEC phenomenon was observed directly in dilute vapors of alkali atoms, such as rubidium [3], lithium [4], and sodium [5], confined in magnetic traps and cooled down to nanokelvin temperatures.

These remarkable experimental observations [3-5] have stimulated much activities in experiments [6-11] and in the theoretical investigation of inhomogeneous Bose gases. It is impractical to quote all of numerous theoretical papers published during the past few years. We quote here only a fraction [12-28] of the theoretical papers, which are relevant to this paper and are based mostly on the Ginzburg-Pitaevskii-Gross (GPG) equation (also known as Pitaevskii-Gross (PG) equation) [29-32], which is believed to describe accurately the experimental results well below the onset of BEC. The GPG equation is a nonlinear Schrödinger equation (NLSE), which is formally identical to a Ginzburg-Landau type of field equations (the Ginzburg-Landau theory is also known as ψ theory [36]). The NLSE is one of the nonlinear differential equations, the study of which led to fundamental advances in nonlinear dynamics [37].

Since the vapors used in the experiment are dilute, the average distance between the atoms is substantially larger than the range of the interaction. Hence, the Bose gas is expected to be dominated by two-body collisions, which can be well described by the s-wave scattering length. Thus, the Ginsburg-Pitaevskii-Gross theory developed for weakly interacting bosons is ideally suited to describe BEC observed in the experiments.

The numerical methods based on variational principles (VP) are the most effective approximation method and have been used to solve the GPG equation using the numerical minimization of the energy functional [14, 16, 21, 25, 28]. However, it is expected that the wave function determined by the variational method is much less accurate than the stationary value of the functional itself (e.g. energy), because the later value is only indirectly related to the wave function and depends weakly on the trial wave function near the stationary point. We note in contrast that, for the case of the linear Schrödinger equation, one can obtain the criteria of accuracy not only for stationary quantities but also for the wave function using Schwinger variational principles [35].

In this paper, we present a systematic construction of VP which is free of the above shortcomings, based on the approach proposed by Gerjuoy, Rau, and Spruch (GRS) [36]. We introduce a functional whose optimal value is the wave function at given values of its arguments. In section 2, we give a brief review of the GPG (or PG) equation as it relates to BEC. In section 3, we give an outline of GRS approach for variational principles. Section 4 describes our derivation of a functional, stationary value of which is the chemical potential, and section 5 describes the VP for the wave function. In section 6, we describe our formulation of iteration method based on our VP for the wave function. Summary and conclusions are given in section 7. In the Appendix we describe an example of the application of our variational iteration method to a nonlinear integral equation.

2. Nonlinear Schrödinger Equation

For a dilute gas of bosons at zero temperature mean field theory yields a nonlinear Schrödinger equation (NLSE) for the condensate wave function [32]. The condensate wave function (or order parameter) may be described by a self-consistent mean field NLSE known as the Ginsburg-Pitaevskii-Gross (GPG) equation (also known as Gross-Pitaevskii (GP) equation [29-31]. For condensed neutral atoms in an external trap, the GPG equation takes a form

$$\frac{i\hbar\partial\psi(\vec{r},t)}{\partial t} = \frac{\hbar^2}{2m} \nabla^2\psi(\vec{r},t) + V_{trap}(\vec{r})\psi(\vec{r},t) + V_H(\vec{r})\psi(\vec{r},t) \quad (1)$$

where $\psi(\vec{r}, t)$ is the BEC wavefunction, m is the atom mass, and $V_{trap}(\vec{r})$ is a trap potential. $V_H(\vec{r})$ is the mean Hartree interaction energy for the condensate

$$V_H(\vec{r}) = g_0 N_0 |\psi(\vec{r}, t)|^2, \quad (2)$$

where N_0 is the total number of the BEC atoms, and

$$g_0 = \frac{4\pi\hbar^2 a}{m} \quad (3)$$

with the scattering length a . To obtain a stationary solution, we insert $\psi(\vec{r}, t) = \exp(-i\frac{\mu_0}{\hbar}t)\psi(\vec{r})$ (where μ_0 is the chemical potential) into Eq. (1) to find the following equation for $\psi(\vec{r})$

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V_{trap}(\vec{r})\psi(\vec{r}) + g_0 N_0 |\psi(\vec{r})|^2\psi(\vec{r}) = \mu_0\psi(\vec{r}), \quad (4)$$

$$\int d\vec{r} |\psi(\vec{r})|^2 = 1. \quad (5)$$

For an anisotropic harmonic oscillator trap, $V_{trap}(\vec{r})$ is given by

$$V_{trap}(\vec{r}) = m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/2. \quad (6)$$

In this paper, we develop the variational principles, for solving Eq. (4) based on the approach proposed by Gerjuoy, Rau, and Spruch [36]. The GRS variational principles for the time-dependent Eq. (1) will be given elsewhere.

3. Variational Principles of Gerjuoy, Rau, and Spruch.

In this section, we give a brief outline of the unified formulation of the construction of variational principles, developed by Gerjuoy, Rau, and Spruch GRS [36].

We start with the following set of equations

$$B_i(\phi) = 0, \quad i = 1, 2, \dots, \quad (7)$$

where ϕ designates a set of function are precisely defined by relations (7).

Now, let (ϕ_t, ϕ_t^*) be a trial estimate of exact but unknown (ϕ, ϕ^*) , and let (L_t^i, \tilde{L}_t^i) , be a trial estimate of a (L^i, \tilde{L}^i) to be specified. Then, the functional

$[F] = F_v(\phi_t, \phi_t^*, L, \tilde{L})$ is a variational functional for the desired $F(\phi, \phi^*)$ which we seek, if

$$F_v(\phi, \phi^*, L_t, \tilde{L}_t) = F(\phi, \phi^*), \quad (8)$$

and

$$\delta[F] = F_v(\phi_t, \phi_t^*, L_t, \tilde{L}_t) - F(\phi, \phi^*) = O(\delta\phi^2, \delta L^2, \delta\phi\delta L), \quad (9)$$

where

$$L^i = L_t^i + \delta L^i, \quad \tilde{L}^i = \tilde{L}_t^i + \delta \tilde{L}^i, \quad \phi = \phi_t + \delta\phi, \quad \phi^* = \phi_t^* + \delta\phi^*. \quad (10)$$

Now, consider

$$[F] = F(\phi_t, \phi_t^*) + \sum_i (\langle L_t^i | B_i(\phi_t) \rangle + \langle B_i(\phi_t) | \tilde{L}_t^i \rangle). \quad (11)$$

Using Eqs. (9 - 11) we can determine the necessary relations specifying (L^i, \tilde{L}^i) , whose estimates (L^i, \tilde{L}^i) appear in Eq. (9). The essential point is that there are no restrictions on the nature of $\phi, F(\phi)$, and $B(\phi)$. Therefore the GRS method is a general method for construction of VP for linear, nonlinear, differential, and integral equations.

4. Variational Principle for the Chemical Potential

In this section we derive a functional whose stationary value is the chemical potential μ_0 . We start with Eq. (4)

$$(T + V_{trap} + g_0 N_0 |\psi|^2) \psi = \mu_0 \psi, \quad (4a)$$

where T is the kinetic energy operator

$$T = -\frac{\hbar^2}{2m} \nabla^2. \quad (12)$$

Now, let us consider a functional $[\mu_0]$

$$\begin{aligned} [\mu_0] &= \mu_t + \lambda^t [(\langle \psi_t | \psi_t \rangle - 1) + \langle L_t | (T + V_{trap} + g_0 N_0 |\psi_t|^2 - \mu_t) | \psi_t \rangle \\ &+ \langle (T + V_{trap} + g_0 N_0 |\psi_t|^2 - \mu_t) \psi_t | L_t \rangle], \end{aligned} \quad (13)$$

where

$$\lambda^t = \frac{1}{\langle L_t | \psi_t \rangle + \langle \psi_t | L_t \rangle}, \quad (14)$$

and $L_t(\vec{r})$ is solution of linear equation

$$(T + V_{trap} + 2g_0N_0|\psi_t|^2)L_t + g_0N_0\psi_t^2L_t^* - \mu_tL_t = -\psi_t, \quad (15)$$

with boundary conditions

$$\lim_{r \rightarrow \infty} L_t(\vec{r}) \rightarrow 0. \quad (16)$$

To prove that $[\mu_0]$, Eq. (13) is a stationary expression, let us calculate $\delta[\mu_0]$, let

$$\begin{aligned} \psi_t &= \psi + \delta\psi, \quad \psi_t^* = \psi^* + \delta\psi^*, \\ \mu_t &= \mu_0 + \delta\mu, \quad L_t = L + \delta L. \end{aligned} \quad (17)$$

We also assume that

$$\delta\mu = O(\delta\psi), \quad \delta L = O(\delta\psi). \quad (18)$$

Substitution of Eq. (17) into Eq. (13) gives

$$\begin{aligned} \delta[\mu_0] &= \delta\mu[1 - \lambda(\langle L|\psi\rangle + \langle\psi|L\rangle)] + \\ &\quad \lambda(\langle\delta\psi|\psi\rangle + \langle\psi|\delta\psi\rangle + \langle\delta\psi|(T + V_{trap} + 2g_0N_0|\psi|^2 - \mu_0)|L\rangle + \\ &\quad \langle\delta\psi|g_0N_0\psi^2|L^*\rangle + \langle\psi|(T + V_{trap} + 2g_0N_0|\psi|^2 - \mu_0)L|\delta\psi\rangle + \\ &\quad \langle g_0N_0\psi^2L^*|\delta\psi\rangle) + O(\delta\psi^2). \end{aligned} \quad (19)$$

Using

$$\lambda = (\langle L|\psi\rangle + \langle\psi|L\rangle)^{-1},$$

and Eq. (18), we obtain

$$\delta[\mu_0] = O(\delta\psi^2).$$

Since homogeneous equation

$$(T + V_{trap} + 2g_0N_0|\psi|^2)L + g_0N_0\psi^2L^* - \mu L = 0 \quad (21)$$

has a solution

$$L = ic\psi, \quad (22)$$

where c is a real constant, and there is no homogeneous solution in general of

$$(T + V_{trap} + 2g_0N_0|\psi_t|^2)L_t + g_0N_0\psi_t^2L_t^* - \mu_tL_t = 0, \quad (23)$$

our assumption given by Eq. (18), $\delta L = O(\delta\psi)$, has to be justified. In general, we need to modify Eq. (15). (For the case of the linear Schrödinger equation, see [36]). However, for ground state of the GPG equation, we do

not need to modify Eq. (15). In this case, $\psi_t^* = \psi_t$, and from Eq. (15) we write

$$\begin{aligned} (T + V_{trap} + 2g_0N_0|\psi_t|^2)R_eL_t + g_0N_0|\psi_t|^2R_eL_t - \mu_tR_eL_t &= -\psi_t, \\ (T + V_{trap} + 2g_0N_0|\psi_t|^2)ImL_t - g_0N_0|\psi_t|^2ImL_t - \mu_tImL_t &= 0, \end{aligned} \quad (24)$$

where

$$L_t = ReL_t + iImL_t.$$

For this case, we need to solve Eq. (15) for real solution $L_t (L_t^* = L_t)$ and hence the problem will not arise.

5. Variational principle for wave function

In this section, we attempt to solve the following problem how to find variational estimates of the BEC wave function. To do this, we introduce a functionals $[Re\psi](\vec{r})$ and $[Im\psi](\vec{r})$ whose stationar values are $[Re\psi](\vec{r})$ and $Im\psi(\vec{r})$ respectively

$$\begin{aligned} [Re\psi](\vec{r}) &= \frac{1}{2}(\psi_t(\vec{r}) + \psi_t^*(\vec{r})) - \frac{1}{2} \int L_R^{t*}(\vec{r}, \vec{r}') [T + V_{trap} + g_0N_0|\psi_t|^2 \\ &- \mu_t]\psi_t(\vec{r}') d\vec{r}' - \frac{1}{2} \int [(T + V_{trap} + g_0N_0|\psi_t|^2 - \mu_t)\psi_t(\vec{r})]^* L_R^t(\vec{r}, \vec{r}') d\vec{r}', \end{aligned} \quad (25)$$

$$\begin{aligned} [Im\psi](\vec{r}) &= \frac{1}{2i}(\psi_t(\vec{r}) - \psi_t^*(\vec{r})) - \frac{1}{2i} \int [L_I^{t*}(\vec{r}, \vec{r}') [T + V_{trap} + g_0N_0|\psi_t|^2 - \mu_t]\psi_t(\vec{r}') d\vec{r}' \\ &+ \frac{1}{2i} \int [(T + V_{trap} + U_0N_0|\psi_t|^2 - \mu_t)\psi_t(\vec{r})]^* L_I^t(\vec{r}, \vec{r}') d\vec{r}', \end{aligned} \quad (26)$$

where $L_I^t(\vec{r}, \vec{r}')$, and $L_R^t(\vec{r}, \vec{r}')$ are solutions of linear equations

$$[T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t]L_R^t(\vec{r}, \vec{r}') + g_0N_0\psi_t^2L_R^{t*}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'), \quad (27)$$

$$[T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t]L_I^t(\vec{r}, \vec{r}') - g_0N_0\psi_t^2L_I^{t*}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'). \quad (28)$$

Varying Eqs. (25) and (26) we obtain

$$\begin{aligned} \delta[Re\psi](\vec{r}) &= \int d\vec{r}' \left\{ \frac{1}{2} \{ \delta(\vec{r} - \vec{r}') (\delta\psi(\vec{r}') + \delta\psi^*(\vec{r}')) - \right. \\ &- \frac{1}{2} [(T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t)L_R^t(\vec{r}, \vec{r}')^* \delta\psi(\vec{r}') \\ &+ g_0N_0\psi^{*2}(\vec{r}')L_R^t(\vec{r}, \vec{r}')\delta\psi(\vec{r}') \\ &+ [T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t]L_R^t(\vec{r}, \vec{r}')\delta\psi^*(\vec{r}') \\ &+ g_0N_0\psi^2(\vec{r}')L_R^{t*}(\vec{r}, \vec{r}')\delta\psi^*(\vec{r}')] \} + O(\delta\psi^2), \end{aligned} \quad (29)$$

and

$$\begin{aligned}
\delta[Im\psi](\vec{r}') &= \int d\vec{r} \left\{ \frac{1}{2i} \{ \delta(\vec{r} - \vec{r}') (\delta\psi(\vec{r}) - \delta\psi^*(\vec{r}')) \right. \\
&\quad - \frac{1}{2i} [(T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t) L_I^t(\vec{r}, \vec{r}')^* \delta\psi(\vec{r}) \\
&\quad - g_0N_0\psi^{*2}(\vec{r}') L_I^t(\vec{r}, \vec{r}') \delta\psi(\vec{r}') \\
&\quad - [T + V + 2g_0N_0|\psi|^2 - \mu_t] L_I^t(\vec{r}, \vec{r}') \delta\psi^*(\vec{r}') \\
&\quad \left. + g_0N_0\psi^2(\vec{r}') L_I^{t*}(\vec{r}, \vec{r}') \delta\psi^*(\vec{r}') \} \right\} + O(\delta\psi^2),
\end{aligned} \tag{30}$$

where we have assumed

$$\mu_t = \mu_0 + \delta\mu, \delta\mu = O(\delta\psi^2), \tag{31}$$

and

$$L_{R,I}^t = L_{R,I} + \delta L_{R,I}, \delta L_{R,I} = O(\delta\psi). \tag{32}$$

Substitution of Eqs. (27), (28) into Eqs. (29) and (30) leads to equations

$$\begin{aligned}
\delta[Re\psi](\vec{r}) &= O(\delta\psi^2), \\
\delta[Im\psi](\vec{r}) &= O(\delta\psi^2),
\end{aligned} \tag{33}$$

which prove that Eqs. (25) and (26) are variational functionals.

Using Eqs. (25) and (26) we can derive a variational principle for ψ itself

$$\begin{aligned}
[\psi](\vec{r}) &= [Re\psi](\vec{r}) + i[Im\psi](\vec{r}) = \psi_t(\vec{r}) + \int R_2^{t*}(\vec{r}, \vec{r}') [T + V_{trap} \\
&\quad + g_0N_0|\psi_t|^2 - \mu_t] \psi_t(\vec{r}') d\vec{r}' \\
&\quad + \int [(T + V_{trap} + g_0N_0|\psi_t|^2 - \mu_t) \psi_t(\vec{r}')^* R_1^t(\vec{r}, \vec{r}') d\vec{r}',
\end{aligned} \tag{34}$$

where

$$R_1^t(\vec{r}, \vec{r}') = -\frac{1}{2}(L_R^t(r, r') - L_I^t(r, r')), \tag{35}$$

$$R_2^t(r, r') = -\frac{1}{2}(L_R^t(r, r') + L_I^t(r, r')). \tag{36}$$

It is convenient to rewrite Eq. (34) as follows

$$\begin{aligned}
[\psi](\vec{r}') &= -2 \int \psi_t^*(\vec{r}') g_0N_0|\psi_t(\vec{r}')|^2 R_1^t(\vec{r}, \vec{r}') d\vec{r}' \\
&\quad - 2 \int R_2^{t*}(\vec{r}, \vec{r}') g_0N_0|\psi_t(\vec{r}')|^2 \psi_t(\vec{r}') d\vec{r}'.
\end{aligned} \tag{37}$$

Three comments are appropriate here. First, for the ground state of the GPG equation, we have $\psi_t^* = \psi_t$, and from Eq. (21)

$$\begin{aligned}
[\psi](\vec{r}) &= \int \psi_t(\vec{r}') g_0N_0|\psi_t(\vec{r}')|^2 L_R^t(\vec{r}, \vec{r}') d\vec{r}' \\
&\quad + \int L_R^{t*}(r, r') g_0N_0|\psi_t(\vec{r}')|^2 \psi_t(\vec{r}') d\vec{r}'.
\end{aligned} \tag{38}$$

Secondly, if $L_R(\vec{r}, \vec{r}') = L_R^*(\vec{r}, \vec{r}')$, the following equation

$$[T + V_{trap} + 2g_0N_0|\psi|^2 - \mu_0]L_R + g_0N_0\psi^2L_R^* = \delta(\vec{r} - \vec{r}') \quad (39)$$

has a unique solution, since in this case the homogeneous equation has only a trivial solution.

Thirdly, if $\psi_t^* \neq \psi_t$ (vortex states), Eqs. (27) and (28) are meaningless. To see this, we use Eqs. (27), (28), (35), and (36) to obtain

$$\begin{aligned} (T + V_{trap} + 2g_0N_0|\psi|^2 - \mu_0)R_2 + g_0N_0\psi^2R_1^* &= -\delta(\vec{r} - \vec{r}'), \\ (T + V_{trap} + 2g_0N_0|\psi|^2 - \mu_0)R_1 + g_0N_0\psi^2R_2^* &= 0, \end{aligned} \quad (40)$$

where ψ is exact solution of the GPG equation (4). Multiplying Eqs. (40) on the left by $\psi^*(\vec{r}')$ and integrating, we find, using Eq. (4), that

$$\begin{aligned} \int g_0N_0|\psi(\vec{r}')|^2(\psi^*(\vec{r}')R_2(\vec{r}, \vec{r}') + \psi(\vec{r}')R_1^*(\vec{r}, \vec{r}'))d\vec{r}' &= -\psi(\vec{r}), \\ \int g_0N_0|\psi(\vec{r}')|^2(\psi^*(\vec{r}')R_1(\vec{r}, \vec{r}') + \psi(\vec{r}')R_2^*(\vec{r}, \vec{r}'))d\vec{r}' &= 0. \end{aligned} \quad (41)$$

Eqs. (41) do not have solutions if $\psi(\vec{r}) \neq 0$. As noted in [36], when constructing variational principles for certain quantities (as, for example, for $\psi(\vec{r})$), it is expected that some specification of the phase of the wave function must be imposed; otherwise, various ambiguities and contradictions can occur (see Eqs. (40)). There are various ways of specifying the phase of ψ . The simplest and useful procedure is to fix the phase of ψ relative to some arbitrary known function $\chi(r)$ through a restriction of the sort that $\langle \psi | \chi \rangle$ is either purely real or purely imaginary [36].

Therefore we write

$$\begin{aligned} [\psi](\vec{r}) &= \psi_t(\vec{r}) + \gamma_t(\vec{r})(\langle \psi_t | \chi \rangle - \langle \chi | \psi_t \rangle) + \\ &+ \int R_2^{t*}(\vec{r}, \vec{r}') [T + V_{trap} + g_0N_0|\psi_t|^2 - \mu_t] \psi_t(\vec{r}') d\vec{r}' + \\ &+ \int [(T + V_{trap} + g_0N_0|\psi_t|^2 - \mu_t) \psi_t(\vec{r}')^* R_1^t(\vec{r}, \vec{r}') d\vec{r}', \end{aligned} \quad (42)$$

where

$$\begin{aligned} (T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t)R_2^{t*}(\vec{r}, \vec{r}') + g_0N_0\psi_t^{*2}R_1^t(\vec{r}, \vec{r}') + \\ + \delta(\vec{r} - \vec{r}') - \gamma_t(\vec{r})\chi^*(\vec{r}') = 0, \end{aligned} \quad (43)$$

$$\begin{aligned} (T + V_{trap} + 2g_0N_0|\psi_t|^2 - \mu_t)R_1^t(\vec{r}, \vec{r}') + g_0N_0\psi_t^2R_2^{t*}(\vec{r}, \vec{r}') + \\ + \gamma_t(\vec{r})\chi(\vec{r}') = 0, \end{aligned} \quad (44)$$

$$\gamma_t(\vec{r}) = 0.5\psi_t(\vec{r}) / \langle \psi_t | \chi \rangle, \quad (45)$$

and

$$\langle \psi_t | \chi \rangle = \langle \chi | \psi_t \rangle. \quad (46)$$

Varying Eq. (42) we obtain

$$\delta[\psi](\vec{r}) = O(\delta\psi^2), \quad (47)$$

where we have assumed Eq. (31) and

$$\delta R_i = O(\delta\psi), i = 1, 2 \quad (48)$$

Using Eqs. (43)-(46) we can rewrite Eq. (42) as Eq. (37).

6. Variational-iteration method

To solve nonlinear problems, one frequently uses the method of iteration, several iteration schemes are possible [15, 37].

Now we formulate iteration method which directly follows from variational methods given by Eqs. (37) and (38),

$$\begin{aligned} \psi^{(N)}(\vec{r}) &= \int d\vec{r}' Q_1^{(N-1)}(\vec{r}, \vec{r}') \psi^{(N-1)}(\vec{r}') d\vec{r}' \\ &+ \int d\vec{r}' Q_2^{(N-1)}(\vec{r}, \vec{r}') (\psi^{(N-1)}(\vec{r}'))^* d\vec{r}', \end{aligned} \quad (49)$$

where, for example, for ground state ($\psi^{(N)} = \psi^{(N)*}$),

$$\begin{aligned} Q_1^{(N-1)}(\vec{r}, \vec{r}') &= Q_2^{(N-1)}(\vec{r}, \vec{r}') \\ &= g_0 N_0 \psi^{(N-1)}(\vec{r}') L_R^{(N-1)}(\vec{r}, \vec{r}'). \end{aligned} \quad (50)$$

$L_R^{(N-1)}(r, r')$ is a solution of the linear equation

$$\begin{aligned} [T + V_{trap} &+ 2g_0 N_0 |\psi^{(N-1)}|^2 - \mu^{(N-1)}] L_R^{(N-1)} + g_0 N_0 (\psi^{(N-1)})^2 L_R^{(N-1)} \\ &= \delta(\vec{r} - \vec{r}'), \end{aligned} \quad (51)$$

where

$$\begin{aligned} \mu^{(N-1)} &= \mu_t^{(N-1)} + \lambda^{(N-1)} \langle L^{(N-1)} | T + V_{trap} + g_0 N_0 |\psi^{(N-1)}|^2 - \mu_t^{(N-1)} | \psi^{(N-1)} \rangle, \\ \lambda^{(N-1)} &= 1 / \langle L^{(N-1)} | \psi^{(N-1)} \rangle, \end{aligned} \quad (52)$$

$$\mu_t^{(N-1)} = \langle \psi^{(N-1)} | T + V_{trap} + V_H^{(N-1)} | \psi^{(N-1)} \rangle, \quad (53)$$

with

$$V_H^{(N-1)} = g_0 N_0 |\psi^{(N-1)}(\vec{r})|^2, \quad (54)$$

and $L^{(N-1)}$ is a quadratically integrable solution of the linear nonhomogeneous equation

$$(T + V_{trap} + 3V_H^{(N-1)} - \mu_t^{(N-1)})L^{(N-1)} = -\psi^{(N-1)}. \quad (55)$$

Eqs. (50-55) can be easily generalized to include vortex states. We note that one of the primary motivations of the GPG theory was the study of vortex states in weakly interacting bosons [30, 31]. We expect a super-fast convergence of the iteration process describing by Eqs. (49-55). It follows from the fact that, if $(\psi - \psi^{(N-1)}) = O(\delta\psi)$, then $(\psi - \psi^{(N)}) = O(\delta\psi^2)$.

To simplify the iteration process given by Eqs. (49-55) let us introduce

$$\begin{aligned} \psi^{(N)}(\vec{r}) &= \int d\vec{r}' Q_1^{(0)}(\vec{r}, \vec{r}') \psi^{(N-1)}(\vec{r}') d\vec{r}' \\ &+ \int d\vec{r}' Q_2^{(0)}(\vec{r}, \vec{r}') (\psi^{(N-1)}(r'))^* d\vec{r}'. \end{aligned} \quad (56)$$

This scheme is much simpler than Eqs. (49 - 55) since we need to solve a set of linear equations (51) and (55) only once (for $N = 1$). If function $\psi^{(0)}$ is chosen sufficiently close to ψ , the $Q_i^{(N-1)}(r, r')$ and $Q_i^{(0)}(\vec{r}, \vec{r}')$ will differ only by small amount. This provides the basis for the iteration process given by Eq. (56) [36]. To solve a set of linear equations, Eqs. (51) and (55), we can expand solutions in a basis of anisotropic trap eigenfunctions [15].

$$\begin{aligned} \psi^{(N-1)}(\vec{r}) &= \sum_{i=1}^{N_{basis}} \alpha_i^{(N-1)} \phi_{x_i}(x) \phi_{y_i}(y) \phi_{z_i}(z), \\ L^{(N-1)}(\vec{r}) &= \sum_{i=1}^{N_{basis}} \beta_i^{(N-1)} \phi_{x_i}(x) \phi_{y_i}(y) \phi_{z_i}(z), \\ L_R^{(N-1)}(\vec{r}, \vec{r}') &= \sum_{i,j=1}^{N_{basis}} \gamma_{ij}^{(N-1)} \phi_{x_i}(x) \phi_{y_i}(y) \phi_{z_i}(z) \phi_{x_j}(x') \phi_{y_j}(y') \phi_{z_j}(z'), \end{aligned} \quad (57)$$

where $\phi_{n_i}(y)$ is a one-dimensional harmonic-oscillator eigenfunction. The coefficients, $\alpha_i^{(N-1)}$, $\beta_i^{(N-1)}$, and $\gamma_{ij}^{(N-1)}$, can be expressed in terms of

$$J_{n_i n_j n_k n_l} = \int_{-\infty}^{+\infty} dy \phi_{n_i}(y) \phi_{n_j}(y) \phi_{n_k}(y) \phi_{n_l}(y), \quad (58)$$

which can be evaluated analytically [38].

7. Summary and Conclusions

Based on the GRS approach [36], we have derived variational principles for the nonlinear Schrödinger equation in a systematic way. In particular, we have obtained variational principle for eigenvalues (chemical potential) and wave function of the GPG equation. To the best of our knowledge,

these variational principles for the GPG equation are new. Using these variational principles, we have formulated a variational iteration method, which is expected to have a very fast convergence.

We are planning to generalize our results to the case of nonstationary GPG equation and to carry out relevant numerical calculations based on our method.

Appendix

Our variational iteration method developed in this paper is general and can be applied to both nonlinear differential equation and nonlinear integral equation. In this Appendix, we describe one example of the application of our variational iteration method to non-linear integral equation

$$y(x) = \int_a^b K(x, s, y(s))ds, \quad (x, s) \in [a, b], \quad (A.1)$$

where $K(x, s, y)$ is a continuous function, with all its variables continuous, and has continuous low order derivatives. We introduce a functional $[y](x)$ whose stationary value is $y(x)$

$$[y](x) = \int_a^b K(x, t, y_t(t))dt + \int_a^b L(x, x')[y_t(x') - \int_a^b K(x', t, y_t(t))dt]dx', \quad (A.2)$$

where $L(x, x')$ is solution of a linear integral equation

$$L(x, t) - \int_a^b ds' L(x, s') \frac{\partial K}{\partial y_t}(s', t, y_t(t)) = -\frac{\partial K(x, t, y_t(t))}{\partial y_t}. \quad (A.3)$$

Iteration procedure which follows directly from the variational functional (A.2) is

$$\begin{aligned} y^{(N)}(x) &= \int_a^b K(x, t, y^{(N-1)}(t))dt \\ &+ \int_a^b L^{(N-1)}(x, s)[y^{(N-1)}(s) \\ &- \int_a^b K(s, t, y^{(N-1)}(t))dt]ds, \end{aligned} \quad (A.4)$$

$$L^{(N-1)}(s, t) - \int_a^b dx' L^{(N-1)}(s, x') \frac{\partial K(x', t, y^{(N-1)}(t))}{\partial y^{(N-1)}} = -\frac{\partial K(s, t, y^{(N-1)}(t))}{\partial y^{(N-1)}}. \quad (A.5)$$

The above iteration procedure is equivalent to the Kantorovich-Newton process (KN) [37] which has developed for nonlinear integral equations:

$$y^{(N)}(x) = y^{(N-1)}(x) + \phi_{N-1}(x), \quad (A.6)$$

$$\phi_{N-1}(x) = \epsilon_{N-1}(x) + \int_a^b \frac{\partial K(x, s, y^{(N-1)}(s))}{\partial y^{(N-1)}} \phi_{N-1}(s)ds, \quad (A.7)$$

where

$$\epsilon_{N-1}(x) = \int_a^b K(x, s, y^{(N-1)}(s))ds - y^{(N-1)}(x). \quad (A.8)$$

To show the equivalence between the KN method and our method for solving the nonlinear integral equation (A.1), we rewrite solution of Eq. (A.7) as

$$\phi_{N-1}(x) = \int_a^b \Gamma^{(N-1)}(x, s) \epsilon_{N-1}(s) ds, \quad (A.9)$$

where

$$\Gamma^{(N-1)}(x, t) = \delta(x - t) + \int_a^b \frac{\partial K(x, s, y^{(N-1)}(s))}{\partial y^{(N-1)}} \Gamma^{(N-1)}(s, t) ds. \quad (A.10)$$

Substitution of Eq. (A.9) into Eq. (A.6) gives

$$\begin{aligned} y^{(N)}(x) &= \int_a^b K(x, t, y^{(N-1)}(t)) dt \\ &+ \int_a^b [-ds' \frac{\partial K(x, s', y^{(N-1)}(s'))}{\partial y^{(N-1)}} \Gamma^{(N-1)}(s', s)] (y^{(N-1)}(s) - \\ &- \int_a^b K(s, t, y^{(N-1)}(t)) dt) ds \end{aligned} \quad (A.11)$$

Using Eq. (A.10), we obtain

$$- \int_a^b ds' \frac{\partial K(x, s', y^{(N-1)}(s'))}{\partial y^{(N-1)}} \Gamma^{(N-1)}(s', s) = L^{(N-1)}(x, s) \quad (A.12)$$

Therefore, the KN method developed for the nonlinear integral equation (A.1) is a special case of the GRS approach.

We shall illustrate a numerical convergence of the iteration procedures (A.4)-(A.5) for an example [37] of the following nonlinear integral equation,

$$y(x) = \frac{1}{2} \int_0^1 [y(t)]^2 x t dt + 1. \quad (A.13)$$

The exact solution of this equation has the form

$$y(x) = 1 + ax, \quad (A.14)$$

where a is given as solutions of a quadratic equation. There are two solutions of Eq. (A.9) with $a \approx 0.40589$ and $a \approx 4.92744$.

For case of $y^{(N)} = 1 + a^{(N)}x$, the iteration procedure (A4-A5) reduces to

$$\begin{aligned} a^{(N)} &= [\frac{1}{4} + \frac{1}{3}a^{(N-1)} + \frac{1}{8}(a^{(N-1)})^2][1 - \frac{12}{3a^{(N-1)}-8}(1/3 + \frac{a^{(N-1)}}{4})] \\ &+ \frac{12}{3a^{(N-1)}-8}a^{(N-1)}(\frac{1}{3} + \frac{a^{(N-1)}}{4}). \end{aligned} \quad (A.15)$$

Starting with $a^{(0)} = 0$, let us calculate the differences $\Delta^{(N)}$ defined as

$$\Delta^{(N)} = \frac{a_{exact} - a^{(N)}}{a_{exact}}, \quad (A.16)$$

where

$$a_{exact} = \frac{8}{3} - \left(\left(\frac{8}{3}\right)^2 - 2\right)^{1/2}.$$

The results are summarized in the Table I.

From Table I, we can see a super-fast convergence of the procedure (A4-A5) for the nonlinear integral equation (A.13).

Starting with values of $a^{(0)}$ in range of $0 \leq a^{(0)} \leq 10$, we have calculated the corresponding values of $a^{(N)}$. The results are summarized in the Table II. We note that in general the convergence of iterative procedure depends on initial step. If $a^{(0)}$ is chosen sufficiently close to the exact value we have a super-fast convergence.

Table I

N	0	1	2	3	4
$\Delta^{(N)}$	1	7×10^{-2}	5×10^{-4}	2×10^{-8}	5×10^{-17}

Table II

$a^{(0)}$	$a^{(1)}$	$a^{(2)}$	$a^{(3)}$	$a^{(4)}$	$a^{(5)}$
0	0.37500	0.40568	0.40589	0.40589	0.40589
1	0.30000	0.40352	0.40588	0.40589	0.40589
2	-1.50000	-0.03000	0.37066	0.40562	0.40589
3	10.50000	6.90957	5.39040	4.96679	4.92778
4	5.25000	4.94758	4.92753	4.92744	4.92744
5	4.92857	4.92744	4.92744	4.92744	4.92744
6	5.10000	4.93356	4.92745	4.92744	4.92744
7	5.42308	4.97200	4.92787	4.92744	4.92744
8	5.81250	5.05190	4.93069	4.92745	4.92744
9	6.23684	5.16756	4.93897	4.92747	4.92744
10	6.68182	5.31072	4.95522	4.92761	4.92744

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